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First principles calculations of stability and lithium intercalation potentials of $ZnCo_2O_4$ L.C. YU, J. WU, H. LIU, Chengdu Green Energy and Green Manufacturing Technology R&D Center, Sichuan, 620107, China, Y.N. ZHANG, Chengdu Green Energy and Green Manufacturing Technology R&D Center, Sichuan; Beijing Computational Science Research Center, Beijing, China —
Among the metal oxides, which are the most widely investigated alternative anodes for use in lithium ion batteries (LIBs), binary and ternary tin oxides have received special attention due to their high capacity values. $ZnCo_2O_4$ is a promising candidate as the anode material for LIB, and one can expect a total capacity corresponding to 7.0 - 8.33 mol of recyclable Li per mole of $ZnCo_2O_4$. Here we studied the structural stability, electronic properties, diffusion barrier and lithium intercalation potentials of $ZnCo_2O_4$ through density functional calculations. The calculated structural and energetic parameters are comparable with experiments. Our DFT studies provide insights in understanding the mechanism of lithium ion displacement reactions in this ternary metal oxide.

Yanning Zhang
Chengdu Green Energy and Green Manufacturing
Technology R&D Center, Sichuan, 620107, China

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